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Exact bounds on the order of the maximum clique of a graph

Marco Budinich

Dipartimento di Fisica and INFN, Università di Trieste, Via Valerio 2, 34127 Trieste, Italy

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Abstract

The paper reviews some of the existing exact bounds to the maximum clique of a graph and successively presents a new upper and a new lower bound. The new upper bound is $\omega \leqslant n - \operatorname{rank} \bar{A}/2$, where $\bar{A}$ is the adjacency matrix of the complementary graph, and derives from a formulation of the maximum clique problem in complex space. The new lower bound is $\omega \geqslant 1/(1 - g_{j^*}(\alpha^*))$ (see text for details) and improves strictly the present best lower bound published by Wilf (J. Combin. Theory Ser. B 40 (1986) 113).

Throughout the paper an eye is kept on the computational complexity of actually calculating the bounds. At the end, the various bounds are compared on 700 random graphs.

Keywords: Graph; Maximum clique; Bound

1. Introduction

Given a graph of order n a clique is a subgraph with pairwise adjacent vertices. The *maximum clique problem* asks for *the order* ω of the largest clique and is NP-complete (see. e.g. [17]).

We consider here unweighted, undirected graphs even if most results hold also without these hypotheses. Furthermore, since every undirected graph can be subdivided into connected subgraphs, we discuss only connected graphs.

As a consequence the adjacency matrices A of our graphs are: symmetric, irreducible and $A \geqslant 0$ containing only 0–1 entries. It follows that all the eigenvalues of A are real and there is just one eigenvalue that equals its spectral radius $\rho(A)$: the Perron root λ_P

E-mail address: mbh@trieste.infn.it (M. Budinich).
URL: http://www.ts.infn.it/~mbh/MBHgeneral.html

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(see e.g. [9, p. 507 ff.]). Moreover, there may be at most just another of the eigenvalues $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{n-1} \leqslant \lambda_P$ with the same modulus, $\lambda_1 = -\lambda_P$, and this happens *if and only if* the graph is bipartite (see [6, Theorems 3.11 and 3.4]). The components of the only eigenvector of λ_P, the Perron eigenvector $\mathbf{x}_P$, are strictly positive i.e. $\mathbf{x}_P > 0$.

The quadratic form $\mathbf{x}'A\mathbf{x}$ ($'$ indicates transposition) is bounded by

$$0 \leqslant \mathbf{x}'A\mathbf{x} \leqslant 1 - \frac{1}{n} \quad \text{when } \mathbf{x} \in K_n = \{\mathbf{x} \in \mathbb{R}^n\colon \mathbf{x} \geqslant 0 \text{ and } \mathbf{e}'\mathrm{x} = 1\},$$

where $\mathbf{e}' = (1, 1, \ldots, 1)$.

A subgraph with q vertices is uniquely determined by its characteristic vector, that is an n-dimensional vector whose ith component, by taking values $1/q$ or 0, indicates whether the ith element belongs or not to the subgraph. Characteristic vectors belong to the simplex K_n.

In 1965 Motzkin and Straus [14] proved the following

Theorem 1. *If the maximum clique of graph A has ω vertices then*

$$\max_{\mathbf{x}\in K_n} \mathbf{x}'A\mathbf{x} = 1 - \frac{1}{\omega}$$

and if $\mathbf{x}_\omega$ is the characteristic vector of a maximum clique then $\mathbf{x}'_\omega A\mathbf{x}_\omega = 1 - 1/\omega$.

Bomze [2] sharpened this result showing that $\max_{\mathbf{x}\in K_n} \mathbf{x}'(A + \frac{1}{2}I)\mathbf{x} = 1 - \frac{1}{2}\omega$ and, moreover, that this quadratic form reaches its maximum if and *only if* $\mathbf{x}$ is the characteristic vector of a maximum clique.

In this formulation the, essentially combinatorial, maximum clique problem is transposed to the search of the maximum of a quadratic function in a bounded region: a continuous optimization problem with linear constraints. Several authors [8,16,18] exploited this formulation to find approximate solutions.

2. Upper bounds

The first upper bound for ω is simple: let m be the number of edges of the graph and $\delta = 2m/n^2$ the density of 1's in A (for connected graphs $2(n-1)/n^2 \leqslant \delta \leqslant (n-1)/n$). The request that a graph, with a clique of ω vertices, is connected gives [1]

$$\omega \leqslant \frac{3 + \sqrt{9 - 8(n-m)}}{2} \tag{1}$$

An upper bound, appeared for the first time in 1967 [19], is

$$\omega \leqslant \rho(A) + 1 \tag{2}$$

the equality holding if and only if the graph is complete. To prove it let $\mathbf{x}_\omega$ be the characteristic vector of a maximum clique, then $\mathbf{x}'_\omega\mathbf{x}_\omega = 1/\omega$ and $\mathbf{x}'_\omega A\mathbf{x}_\omega = 1 - 1/\omega$.

Bound (2) derives from the general property $(\mathbf{x}'A\mathbf{x})/(\mathbf{x}'\mathbf{x}) \leqslant \rho(A)$. With (2) one can apply to ω all the bounds of $\rho(A)$. [1]

The Perron root (and eigenvector) needed for this bound can be easily calculated numerically exploiting the exponentially fast convergence of $\lim_{m\to\infty}(1/\lambda_P)A^m = \mathbf{x}_P\mathbf{x}'_P$ valid if A is primitive (when this is not the case one takes the primitive matrix $A+\frac{1}{2}I$). Successive squaring of A performs this calculation in $O(n^3)$ [9].

Let N_{-1} be number of eigenvalues of A that are less or equal to -1, Amin and Hakimi [1] proved that

$$\omega \leqslant N_{-1} + 1 < \operatorname{rank} A + 1, \tag{3}$$

the equality holding if the graph is complete multipartite.

While bound (1) can be calculated in $O(m) = O(n^2)$, bounds (2) and (3) require $O(n^3)$ but are usually tighter as confirmed by numerical examples at the end of the paper. [2]

We present now a new upper bound based on a property of complex space.

Proposition 1. *Given a graph of order n let $\bar{A}$ be the adjacency matrix of the complementary graph, then*

$$\omega \leqslant n - \frac{\operatorname{rank}\bar{A}}{2}. \tag{4}$$

Proof. Let us suppose that the maximum clique of our graph has order ω and characteristic vector $\mathbf{x}_\omega$; then $\mathbf{x}_\omega$ identifies also a maximum independent set of $\bar{A}$ and thus $\mathrm{x}'_\omega\bar{A}\mathrm{x}_\omega = 0$ (see e.g. [12,17]).

Any real symmetric (not Hermitian) matrix, like $\bar{A}$, may be expressed in the form [9]

$$\bar{A} = B'B = BB = B^2,$$

where B is a complex, symmetric matrix, with the same rank of $\bar{A}$, that we can think formed by n complex column vectors $\mathbf{z}_i \in \mathbb{C}^n$:

$$B = (\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n) \qquad \bar{a}_{jk} = (B'B)_{jk} = \mathbf{z}'_j\mathbf{z}_k$$

[1] This is a partial list of upper bounds for $\rho(A)$:

Upper bound	Reference	Comments
$\max_i \sum_j A_{ij}$	E.g. [9]	Obvious, general bound (valid also for ω); there exists a bound [15] that is sharper by an exponentially small factor
$n\sqrt{\delta} = \sqrt{2m}$	[11]	Since $n\delta \leqslant \lambda_P$ shows that λ_P is $O(n)$
$\sqrt{2m\frac{n-1}{n}}$	[19]	A little tighter than previous one
$\sqrt{2m-n+1}$	[21]	A tighter bound for irreducible matrices

[2] For completeness we mention a different kind of upper bound deriving from the 'Sandwich theorem' reviewed by Knuth [12]. The theorem states that the (polynomially computable) Lovász number of the complementary graph $\bar{\theta}$ is sandwiched between the two NP-hard quantities ω and χ, the chromatic number of the graph, namely, $\omega \leqslant \bar{\theta} \leqslant \chi$. This theorem shows also why, for perfect graphs (for which $\omega = \chi$), ω can be computed in polynomial time.

for which $\mathbf{z}'_i\mathbf{z}_i = \mathbf{z}_i^2 = a_{ii} = 0$. Because of this property, theoretical physicists use to call them *null vectors*, even if length is usually associated to $\mathbf{z}_i^*\mathbf{z}_i$.

The characteristic vector $\mathbf{x}_k$, identifying the nodes $\{j_1, j_2, \ldots, j_\omega\}$ of the maximum independent set of $\bar{A}$, identifies also a subset of the vectors $\mathbf{z}$ that, beyond being null, are also all mutually orthogonal because for any two of them $\mathbf{z}'_{j_i}\mathbf{z}_{j_k} = (B'B)_{j_i j_k} = \bar{a}_{j_i j_k} = 0$.

The span of a set of mutually orthogonal null vectors form a *totally null plane* the so-called because any linear combination of the given vectors is still a null vector. In 1937 Élie Cartan proved [4] that the dimension of any totally null plane contained in $\mathbb{C}^n$ is at most $n/2$.

In our case let $d \leqslant \omega$ be the dimension of the span of the ω complex vectors $\{\mathbf{z}_{j_1}, \mathbf{z}_{j_2}, \ldots, \mathbf{z}_{j_\omega}\}$ and r be the size of the null space of $\bar{A}$ and consequently of B. d is minimum when exactly r of the complex vectors $\mathbf{z}_{j_i}$ belong to the null space of B i.e. we have $\omega - r \leqslant d$. Given the properties of $\bar{A}$ we have $r = n - \operatorname{rank}\bar{A}$ that, together with Cartan's theorem, here giving $d \leqslant \operatorname{rank}\bar{A}/2$, proves bound (4). □

Needing only the rank of $\bar{A}$ this bound can be calculated in $O(n^3)$ and in practice it requires the very same amount of calculations as (3). One can easily find examples in which bounds (2)–(4) are respectively the best;[3] in the last section we compare them on random graphs.

3. Lower bounds

Bounding ω from below is in general harder. Before discussing exact lower bounds we observe that any algorithm that finds cliques can actually provide bounds that, in practical cases, are often easier to calculate and sharper than any exact bound. Unfortunately, these algorithmic bounds tend to take advantage from particular properties of the graph at hand and, in general, have a quite unpredictable behavior: one can easily devise graphs that fool them. On the other hand, exact bounds are usually harder to calculate but rest on vary general properties that frequently provide insights into the problem itself.

The first simple bound derives from the Motzkin and Straus theorem applied to the characteristic vector of the whole graph $\mathbf{e}/n$, i.e. $(\mathbf{e}'A\mathbf{e})/n^2 = 2m/n^2 \leqslant 1 - 1/\omega$ that gives

$$\omega \geqslant \frac{1}{1-\delta}. \tag{5}$$

[3] e.g. for $A = \begin{pmatrix} 0&1&1&0&0&0\\ 1&0&1&1&1&0\\ 1&1&0&0&1&1\\ 0&1&0&0&1&0\\ 0&1&1&1&0&1\\ 0&0&1&0&1&0 \end{pmatrix}$ the sharpest bound is (4).

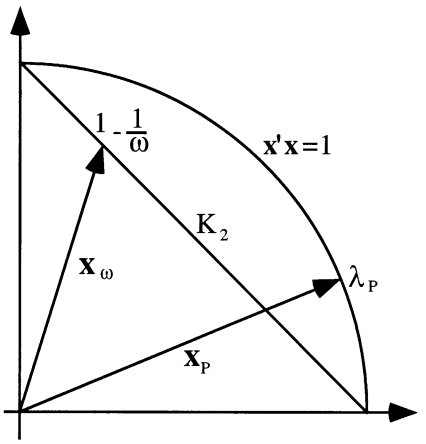

Fig. 1. A schematic drawing in two dimensions.

To get tighter results one needs more powerful instruments: all the results that follow will use spectral graph properties, thus contributing to sustain this promising approach [5]. Wilf [20] improved this and previous bounds [7] applying Motzkin and Straus theorem to the Perron eigenvector divided by $s_P = (\mathbf{e}'\mathbf{x}_P)$ to project it on K_n i.e. $(\mathbf{x}'_P A\mathbf{x}_P)/s_P^2 = \lambda_P/s_P^2 \leqslant 1 - 1/\omega$ thus obtaining

$$\omega \geqslant \frac{\lambda_P}{s_P^2 - \lambda_P} + 1 \geqslant \frac{\lambda_P}{n - \lambda_P} + 1 > 1 \tag{6}$$

equality holding if and only if the graph is complete. The second and third inequalities easily derives from properties of λ_P.

Bounds (2) and (6) have a geometrical interpretation that is simple to grasp in $\mathbb{R}^2$ where both simplex K_2 and the hypersphere $\mathbf{x}'\mathbf{x} = 1$ are one dimensional (see Fig. 1). The absolute maxima of the quadratic form $\mathbf{x}'A\mathbf{x}$ are, respectively, λ_P on the hypersphere and $1 - 1/\omega$ on the simplex. Upper bound (2) is obtained "extending" the characteristic vector of the maximum clique $\mathbf{x}_\omega$ to the hypersphere and bounding the quadratic form with λ_P while the lower bound (6) is obtained "shrinking" the Perron eigenvector $\mathbf{x}_P$ to the simplex and bounding the quadratic form with $1 - 1/\omega$. One can conjecture that the nearer $\mathbf{x}_P$ and $\mathbf{x}_\omega$ the tighter will be the bounds (like in the case of the complete graph where both the two vectors and the two bounds coincide).

To obtain a new bound we followed this conjecture and, starting from $\mathbf{x}_P$ we found a "better" vector $\mathbf{y}$ obtained combining linearly $\mathbf{x}_P$ with another eigenvector $\mathbf{x}_j$. It is always possible to do so remaining within the simplex since $\mathbf{x}_P > 0$ and we will prove that this procedure gives a tighter lower bound.

Let

$$\mathbf{y}_j(\alpha) = \alpha\mathbf{x}_j + \sqrt{1-\alpha^2}\mathbf{x}_P \begin{cases} -1 \leqslant \alpha \leqslant 1, \\ j = 1, \ldots, n-1, \end{cases}$$

by construction: $\mathbf{y}'_j(\alpha)\mathbf{y}_j(\alpha)=1$ and $\mathbf{y}'_j(\alpha)A\mathbf{y}_j(\alpha)=\alpha^2\lambda_j+(1-\alpha^2)\lambda_{\mathrm{P}}$. To use Motzkin and Straus theorem on $\mathbf{y}_j(\alpha)$ it must belong to K_n and we need the following

Proposition 2. *For every eigenvector* $\mathbf{x}_j \neq \mathbf{x}_{\mathrm{P}}$ *let*

$$a_j = \max_{i\,:\,x_{ji}>0} \frac{-x_{\mathrm{P}i}}{\sqrt{x_{\mathrm{P}i}^2+x_{ji}^2}}, \qquad b_j = \min_{i\,:\,x_{ji}<0} \frac{x_{\mathrm{P}i}}{\sqrt{x_{\mathrm{P}i}^2+x_{ji}^2}},$$

then the closed interval $[a_j,b_j]$ *contains the origin in its proper interior and when* $\alpha\in[a_j,b_j]$ *then* $\mathbf{y}_j(\alpha)>0$.

Proof. To prove that $-1<a_j<0<b_j<1$ holds for every j, it is sufficient to observe that every non-zero eigenvector $\mathbf{x}_j$, being orthogonal to $\mathbf{x}_{\mathrm{P}}$, must contain at least one strictly positive and one strictly negative coordinates. From the analytic expressions of a_j and b_j and $\mathbf{x}_{\mathrm{P}}>0$ easily follows that $\mathbf{y}_j(\alpha)>0$ for $\alpha\in[a_j,b_j]$. □

When $\alpha\in[a_j,b_j]$ then $\mathbf{y}_j(\alpha)/(\mathbf{e}'\mathbf{y}_j(\alpha))\in K_n$ and we can use Motzkin and Straus theorem to get

$$\frac{\mathbf{y}'_j(\alpha)}{\mathbf{e}'\mathbf{y}_j(\alpha)} A \frac{\mathbf{y}_j(\alpha)}{\mathbf{e}'\mathbf{y}_j(\alpha)} = \frac{\alpha^2\lambda_j+(1-\alpha^2)\lambda_{\mathrm{P}}}{(\alpha s_j+\sqrt{1-\alpha^2}s_{\mathrm{P}})^2} := g_j(\alpha) \leqslant 1-\frac{1}{\omega},$$

where $s_j=\mathbf{e}'\mathbf{x}_j$. The function $g_j(\alpha)$ is defined for $\alpha\in[a_j,b_j]$ and $g_j(0)=\lambda_{\mathrm{P}}/s_{\mathrm{P}}^2\leqslant 1-1/\omega$ returns Wilf's lower bound (6). In the next proposition we show that this lower bound is not a local optimum.

Proposition 3. *Unless the graph is regular complete multipartite there always exist* j^* *and* α^* *such that* $\max_{j,\alpha} g_j(\alpha)=g_{j^*}(\alpha^*)>g_{j^*}(0)$ *and lower bound* (6) *is strictly sharpened to*

$$\omega \geqslant \frac{1}{1-g_{j^*}(\alpha^*)}. \tag{7}$$

Proof. We start observing that the exclusion of complete multipartite regular graphs is marginal since for these graphs $\omega=N_{-1}+1$ (3). We will demonstrate the propositions showing that if $g_j(0)=\max_{\alpha\in[a_j,b_j]} g_j(\alpha)$ for all j, then the graph is complete multipartite and regular. The request that $g_j(0)$ is maximum for all j needs the vanishing of all the first derivatives i.e.

$$g'_j(\alpha)|_{\alpha=0} = -2\frac{\lambda_{\mathrm{P}}}{s_{\mathrm{P}}^3}s_j = 0$$

satisfied if and only if $s_j=0$ for $j=1,\ldots,n-1$. This in turn means that all eigenvectors $\mathbf{x}_j$ are orthogonal to $\mathbf{e}$ and, since the adjacency matrix is diagonalizable and has a complete set of eigenvectors, $\mathbf{e}$ must also be an eigenvector and precisely the Perron vector. It is known that this happens only for regular graphs (see [6, p. 104]).

The other condition needed to have maximum for $\alpha=0$ concerns the second derivative

$$g_j''(\alpha)|_{\alpha=0} = 2\frac{3\lambda_P s_j^2 + \lambda_j s_P^2}{s_P^4} \leqslant 0$$

and it is easy to verify that when both conditions are met then $\lambda_j \leqslant 0$ for $j=1,\ldots,n-1$. This means that the only positive eigenvalue is the Perron root and this is a necessary and sufficient condition for the graph to be complete multipartite [6, Theorem 6.7]. □

From the expressions of the derivatives of $g_j(\alpha)$ it is easy to see that each eigenvector with $s_j \neq 0$ or $s_j = 0$ and $\lambda_j > 0$ improves the lower bound (6); by checking all these eigenvectors one gets the best-possible improvement.

To calculate numerically the new bound, one first needs the full set of eigenvectors of the adjacency matrix; afterwards it is an $O(n)$ process to find $\max_{j,\alpha} g_j(\alpha)$. So the global computational complexity is dominated by that of the eigendecomposition of the adjacency matrix, that, for a given precision, it is widely believed to be $O(n^3)$ ([3], for a discussion see [13]).

4. Numerical comparisons

To compare quantitatively the various bounds, and in particular the new ones, we decided to test them on 700 random graphs of order $n = 100$ and 200 in place of the more customary DIMACS graphs [10]. There are two reasons to do that: the first is that DIMACS graphs tend to be rather particular and the bounds work rather differently on them and the second is that not all the bounds can be evaluated easily on the largest graphs.

In particular, we generated 50 graphs for each of the selected densities in $0.05 \leqslant \delta \leqslant 0.95$ and for each graph we evaluated exactly ω to check it against the various bounds. Table 1 summarizes these results reporting, for each bound, the ratio of its value over ω. Each table entry represents the average of the ratios obtained for 50 different random graphs; bold figures signal the best bound (on average). For graphs with $n = 200$ and $\delta = 0.9$ the maximum cliques were too hard to calculate and so the table reports the values of the bounds themselves.

For this sample of random graphs upper bounds (2) and (3) are on average lower, but there are 22 cases in which bound (4) is strictly the best.[4] Among lower bounds, bound (7) is always the sharpest as expected. On average, the ratios $bound/\omega$ for (6) are 2% higher than for bound (5) while those of bound (7) are 5% higher than for bound (6).

All numerical calculations have been performed on a portable Mac with Mathematica; the average running time to obtain the lower bounds for graphs or order 100 is 0.32 s. The code was highly non-optimized and more than 99% of the time was expended in the eigendecomposition of the adjacency matrix. Similar results hold for the upper

[4] More precisely, 17 of them are graphs of order 100 and $\delta = 0.95$ and the other 5 are graphs of order 200 and density $\delta = 0.9$ so that the bound seems to be effective for very dense graphs.

Table 1
The bounds evaluated for 700 random graphs; $\bar{\omega}$ indicates the value of ω averaged for the 50 random graphs generated for each n and δ

Random graph			Upper bounds				Lower bounds		
n	δ	$\bar{\omega}$	(1)	(2)	(3)	(4) new	(5)	(6)	(7) new
100	0.05	3.10	6.06	**2.25**	11.58	16.25	0.342	0.352	**0.359**
	0.10	3.98	7.48	**2.99**	10.26	12.58	0.279	0.286	**0.293**
	0.20	5.00	8.75	**4.33**	8.84	10.00	0.250	0.255	**0.262**
	0.30	6.10	8.91	**5.17**	7.52	8.21	0.234	0.239	**0.247**
	0.40	7.54	8.38	**5.49**	6.24	6.66	0.221	0.225	**0.235**
	0.50	9.12	7.72	5.58	**5.19**	5.49	0.217	0.221	**0.232**
	0.60	11.56	6.71	5.28	**4.16**	4.34	0.214	0.218	**0.231**
	0.70	14.58	5.74	4.85	**3.33**	3.44	0.224	0.228	**0.244**
	0.80	19.98	4.48	4.03	**2.45**	2.51	0.241	0.246	**0.266**
	0.90	30.68	3.10	2.94	**1.61**	1.63	0.299	0.305	**0.338**
	0.95	43.52	2.24	2.19	**1.16**	1.16	0.388	0.394	**0.438**
200	0.10	4.16	14.79	**5.25**	20.97	24.20	0.269	0.272	**0.275**
	0.50	11.00	12.84	9.19	**8.71**	9.10	0.181	0.183	**0.189**
	0.90	-	189.69	180.17	**99.10**	100.00	9.558	9.648	**10.320**

bounds. The maximum order of graphs that have been studied in 700. One can expect to gain substantially in all respects with a more dedicated software.

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